CHARTER FOR THE ADVANCED SIMULATION CAPABILITY FOR ENVIRONMENTAL MANAGEMENT (ASCEM) INITIATIVE

PURPOSE

The National Academy of Sciences¹ prioritized the following four research and development gaps for DOE EM's groundwater and soil remediation roadmap:

GS#	Gap	Priority
GS-1	Contaminant behavior in the subsurface is poorly understood.	high
GS-2	Site and contaminant source characteristics may limit the usefulness of baseline subsurface remediation technologies.	medium
GS-3	Long-term performance of trench caps, liners, and reactive barriers cannot be assessed with current knowledge.	medium
GS-4	Long-term ability of cementitious materials to isolate wastes is not demonstrated.	high

The Advanced Simulation Capability for Environmental Management (ASCEM) initiative will address these gaps by developing advanced modeling and simulation capabilities. ASCEM will be a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. This modular and open source high performance computing tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. Use of ASCEM will help EM better estimate cleanup time and costs, and reduce uncertainties and risks.

OBJECTIVES

The objectives of ASCEM are to develop a state-of-the-art, integrated, high-performance computer modeling capability for waste degradation and contaminant release; multi-phase, multi-component, multi-scale subsurface flow and contaminant transport; and environmental exposure and risk assessment, with advanced systematic uncertainty analyses, to support the next generation of performance assessments for groundwater and soil cleanup and waste tank closure activities across the EM complex. Specifically, ASCEM will:

- Simulate coupled processes (hydrological, geochemical, microbiological, & geomechanical)
- Develop graded, iterative and modular toolsets to accurately represent complex EM sites
- Include engineered barrier and waste form degradation, flow and transport, and environmental exposure. Incorporate evaluation of waste staging/area closure in support of closure of waste tank farms.
- Implement formal uncertainty quantification and decision tool analysis in a standardized framework

¹ NATIONAL RESEARCH COUNCIL, Advice on the Department of Energy's Cleanup Technology Roadmap, Gaps and Bridges. The National Academy Press (2009).

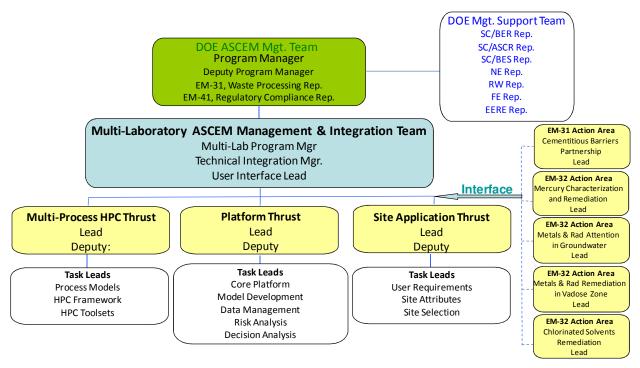
- Implement the capability to be portable from laptops to supercomputers
- Collaborate with user community to demonstrate ASCEM at EM sites
- Verify and validate with site performance data based on scientific understanding of subsurface processes

ORGANIZATION AND MANAGEMENT

ASCEM is a multi-institution, multi-discipline program that is planned and implemented through collaboration of national laboratories and guided by DOE EM Headquarters. The program will involve the best available technical capabilities in hydrogeological, materials, computational, and environmental remediation sciences from DOE national laboratories, leading universities, and private industry. An organization chart for the ASCEM program is shown in Figure 1. Roles and responsibilities of the key organizations and personnel are as follows.

- 1) DOE retains responsibility and authority for developing advanced simulation capabilities for EM within the Office of Technology Innovation & Development (EM-30). The DOE ASCEM Program Manager has the overall responsibility for management and oversight of ASCEM.
- 2) A representative from the Carlsbad Field Office (CBFO) will serve as the Deputy DOE ASCEM Program Manager, and be responsible for oversight of the multi-lab team's interactions with the performance assessment and other user communities within EM. The Deputy will also contribute to the oversight of the project controls functions.
- 3) The DOE ASCEM management team may also include representatives from the EM Office of Regulatory Compliance (EM-41), Office of Waste Processing (EM-31), and other selected EM field offices.
- 4) A DOE management support team will provide technical support to the DOE ASCEM program manager on the planning and reviews of ASCEM activities. Members of this support team may include representatives from DOE Offices of Biological and Environmental Remediation (BER), Advanced Scientific Computing Research (ASCR), Basic Energy Sciences (BES) of the Office of Science (SC); Office of Nuclear Energy (NE); Office of Civil Radioactive Waste Management (RW); Office of Fossil Energy (FE); and Office of Energy Efficiency & Renewable Energy (EERE).
- 5) The participating laboratories will nominate the multi-lab ASCEM project management and integration (M&I) team for DOE approval. The multi-lab M&I team will consist of a dedicated Multi-lab Program Manager (MPM), a Technical Integration Manager (TIM), Technical Thrust Area Leads (TALs), and a User Community Interface Lead. The multi-lab M&I team, with support from the project operations staff (i.e., communications, project controls, and QA), will assure effective project management, including disciplined project planning, execution, reporting, and change control. Together, the M&I team will assure that the project is planned and implemented effectively to deliver the desired outcomes on schedule.
- 6) The MPM provides the single point of contact and overall interface responsibility to the DOE ASCEM Program Manager, and is responsible for the overall coordination of the multi-lab team, including business operation, project controls, QA, and communications.

- 7) The TIM provides overall project technical leadership and is responsible for technical integration across the technical thrusts and with other Federal programs. The TIM is also the lead ASCEM Multi-lab person responsible for providing technical leadership and representation of the project.
- 8) The TALs, supported by their deputies, are responsible for technical leadership, planning and execution of the scope within their designated thrusts and for identifying cross-cutting technical issues.
- 9) The Task Leads and Principal Investigators are responsible, with guidance from the TAL, for their respective tasks at each lab and for fostering an environment of cooperation and coordination with their counterparts at the other ASCEM participating labs.
- 10) The User Community Interface Lead serves as primary project interface with the User Community, to collect input on practical programmatic and regulatory requirements for ASCEM platform, modules, and applications.



Notes:

EM-31: Office of Waste Processing

EM-32: Office of Groundwater and Soil Remediation

SC/BER: DOE Office of Science, Office of Biological and Environmental Remediation

SC/BES: DOE Office of Science, Office of Basic Energy Sciences

SC/ASCR: DOE Office of Science, Office of Applied Scientific Computing Research

NE: DOE Office of Nuclear Energy

RW: DOE Office of Civilian Radioactive Waste Management

FE: DOE Office of Fossil Energy

EERE: DOE Office of Energy Efficiency and Renewable Energy

Figure 1. ASCEM Team Organization.